

MAGE - a GEANT4-based Monte Carlo framework for low-background experiments

Yuen-Dat Chan¹, Jason A. Detwiler^{1,2}, Reyco Henning^{1,3}, Victor M. Gehman^{2,4}, Rob A. Johnson², David V. Jordan⁵, Kareem Kazkaz^{2,6}, Markus Knapp⁷, Kevin Kröninger^{8,9}, Daniel Lenz⁸, Jing Liu⁸, Xiang Liu⁸, Michael G. Marino², Akbar Mokhtarani¹, Luciano Pandola¹⁰, Alexis G. Schubert², Claudia Tomei¹⁰

Abstract—A Monte Carlo framework, MAGE, has been developed based on the GEANT4 simulation toolkit. Its purpose is to simulate physics processes in low-energy and low-background radiation detectors, specifically for the MAJORANA and GERDA ^{76}Ge neutrinoless double-beta decay experiments. This jointly-developed tool is also used to verify the simulation of physics processes relevant to other low-background experiments in GEANT4. The MAGE framework contains simulations of prototype experiments and test stands, and is easily extended to incorporate new geometries and configurations while still using the same verified physics processes, tunings, and code framework. This reduces duplication of efforts and improves the robustness of and confidence in the simulation output.

Index Terms—Monte Carlo, neutrinoless double-beta decay, HPGe detectors, Geant4, radiation detection.

¹ Lawrence Berkeley National Laboratory, Berkeley, CA, USA, ² University of Washington, Seattle, WA, USA, ³ University of North Carolina, Chapel Hill, NC, USA, ⁴ Los Alamos National Laboratory, Los Alamos, NM, USA ⁵ Pacific Northwest National Laboratory, Richland, WA, USA ⁶ Present address: Lawrence Livermore National Laboratory, Livermore, CA, USA, ⁷ Physikalisches Institut, Universität Tübingen, Germany, ⁸ Max-Planck-Institut für Physik, Munich, Germany ⁹ Present address: II. Institute of Physics, University of Göttingen, Germany, ¹⁰ INFN, Laboratori Nazionali del Gran Sasso, Assergi, Italy.

I. INTRODUCTION

MAGE (MAJORANA-GERda) is a GEANT4-based [1], [2] Monte Carlo framework jointly developed by the MAJORANA [3] and GERDA [4] collaborations. Both experiments will search for the neutrinoless double-beta decay ($0\nu\beta\beta$ -decay) of the ^{76}Ge isotope using arrays of HPGe detectors. $0\nu\beta\beta$ -decay is a second-order weak process, the discovery of which is the only practical way to determine if the neutrino is a Majorana particle (for details, see the review article in [5]). The purpose of MAGE is to simulate the MAJORANA and GERDA experiments and their prototypes within a unified coding framework. In the prototyping phase, the simulation is used as a virtual test stand to guide detector design, to estimate the effectiveness of proposed background reduction techniques, and to project the experimental sensitivity. MaGe is used to develop detailed background models, and to study signal characteristics and systematic uncertainties. The simulation is also heavily employed in detector characterization and calibration tasks. The unified framework allows the reuse of code

and verified simulated physics processes. The list of implemented physics models, the so-called physics list in GEANT4, was optimized in MAGE for low-background, underground physics applications [6], with an emphasis on low-energy interactions and hadronic interactions resulting from cosmic ray spallation.

The MAGE concept is discussed in Section II. The code structure (Section III) is followed by the implemented physics list (Section IV). The code is validated by the comparison of data from a variety of test stands and auxiliary experiments with the results of accompanying simulations performed with MAGE. An example for the application of MAGE is presented in Section V. A summary of the validation is given in Section VI. Conclusions are in the last section.

II. CONCEPT

The main goal of the development of MAGE is the creation of a robust, reliable and general-purpose Monte Carlo framework suitable for the simulation of physics processes and background sources relevant for low-background experiments, specifically $0\nu\beta\beta$ -decay experiments.

The structure of the framework allows (1) a parallel and independent development of different branches of the code, for instance geometries and interfaces; (2) ease of maintenance over the full life time of the experiments; and (3) performing simulations with different configurations by nonexperts. The flexibility of MAGE stems from the object-oriented nature of C++ and the GEANT4 toolkit. The MAGE framework provides a single executable. The simulation can be configured (geometry, I/O interface, etc.) with text

file macros. The macros are based on the GEANT4 messenger which allows users to run MAGE in different configurations without editing and recompiling the code. MAGE can thus be run without expert knowledge of the software without restricting its flexibility.

The choice of GEANT4 as the basis for MAGE was motivated by its flexibility and ambitious development within the particle and medical physics communities. A wide number of physics models are included and maintained in GEANT4. The most stringent requirements for MAGE are the proper simulation of the relevant background sources for $0\nu\beta\beta$ -decay experiments. Specifically, this requires a precise description of

- 1) electromagnetic interactions from electrons and γ -rays at MeV and keV energies;
- 2) radioactive isotope decay chains and nuclear de-excitation;
- 3) interactions of thermal and fast neutrons;
- 4) the development of electromagnetic and hadronic showers initiated by cosmic ray muons;
- 5) penetration depths and ionization energy loss profiles of α -particles.

GEANT4 includes specific models for low-energy electromagnetic physics [7], for neutrons below 20 MeV, and for the description of hadronic interactions resulting from cosmic ray spallation. Furthermore, different models in the physics list, tailored to fit specific physics applications (e.g. the simulation of radioactive and muon-induced background contributions) can be selected at runtime using macro commands. The same feature applies to many important tuning parameters, such as the production cuts for δ -rays and soft bremsstrahlung photons. Specific details of the

physics lists implemented in MAGE are discussed in Section IV. The MAGE code is regularly updated and ported in order to make it compatible with the most recent GEANT4 releases, which include new functionalities, improvements and bug fixes.

A further feature of MAGE is the existence of interfaces to other software. MAGE interfaces to external event generators and databases, the latter used to store information about detectors and materials. Furthermore, waveform generators use the output of MAGE to calculate realistic electronic pulses from germanium detectors and hence provide an end-to-end simulation of the experiments. Pulse-shape analysis (PSA) of these pulses allows for powerful background reduction techniques. Monte Carlo simulations are used extensively to test PSA algorithms and other such analysis routines, and to estimate their systematic uncertainties. An end-to-end simulation like MAGE is also an indispensable tool for studying event topologies and problem cases. MAGE also has an abstract output interface that allows event data to be saved in ROOT [8], AIDA-compliant [9], or text-based formats. Therefore MAGE maintains the ability to interface to external analysis tools.

III. STRUCTURE OF MAGE

The structure of MAGE and GEANT4 makes use of the abstraction and object-oriented nature of C++. This allows the user to select the required functionality at runtime by instantiating a class that implements that functionality. The following functionalities can be selected via GEANT4 messengers at runtime:

- **Physics Lists:** A collection of GEANT4 physics processes is called a physics list. They define the particles that are included in the simulation and the

decays and interactions they can undergo. There are several physics lists implemented in MAGE, each optimized for the particular problem being simulated. One list is optimized at higher energies for simulating cosmic-ray muon interactions, while others are optimized for standard electromagnetic interactions at lower energies, i.e. below 10 MeV. These are used to simulate the response of detectors to the decay of radioactive isotopes. Each physics list is contained in its own class that is instantiated at runtime. These lists may have unique associated messengers to further refine the physics processes required.

- **Geometries:** MAGE currently has about 30 user-selectable geometries. Each geometry is encoded in a class that derives from a base class that contains the basic components of a geometry. The user can select a geometry at runtime via messengers. This design also allows the reuse of existing geometry classes, since the classes describing a geometry can be instantiated within a class that requires that component. For example, a detailed germanium crystal has been coded that is used many times in other simulated detector geometries. This crystal can be simulated on its own, or be instantiated many times in a complex detector array. The use of the same basic geometry components eases coding and debugging efforts.
- **Output:** Each detector and Monte Carlo study has unique output requirements. MAGE has several different types of output formats that can be combined to provide the information relevant to a specific study. The base class for output is inherited by classes that add functionality of a specific data

analysis format, such as AIDA, ROOT, or simple text-based output formats. These classes, in turn, are inherited by classes that simulate and store detector responses and save any relevant information. As for the geometries, basic components of the output, such as the readout of a single crystal, can be combined in a single class to create complex detector systems, such as output for the entire MAJORANA or GERDA detector arrays.

- **Event Generators:** GEANT4 provides a suite of tools to create the initial conditions for an event. These include radioactive decay-chain generators and simple volume samplers. MAGE also has the capability to use the GEANT4 RDM [10] generator for radioactive isotope decay. Furthermore it has a custom radioactive decay generator for specific isotopes, such as DECAY0 [11]. This allows for the later inclusion of such effects as angular correlation between emitted γ -rays during ^{60}Co decay, which is not implemented in the RDM generator.

In addition, MAGE includes generators to simulate neutron and muon backgrounds in underground laboratories, using either theoretical models or data-driven approaches. Interfaces are available which read initial conditions for an event from other codes, as SOURCES4A [12] for neutron flux and MUSUN [13] for muon flux.

Additional functionality was added in the form of a complex volume sampler that can generate points uniformly distributed in any GEANT4 boolean solid. This is required to simulate radioactive contamination embedded in detector components. A surface

sampler was also implemented that creates points uniformly distributed on the surface of an arbitrary GEANT4 solid [14]. This is required to simulate surface contaminations, in particular α -emitters. The user selects the appropriate generator at runtime and the corresponding class is instantiated.

- **Materials** MAGE has the ability to read in all relevant information about materials from a PostgreSQL database. This is currently limited to quantities such as density, isotopic abundance, etc. Once the MAJORANA or GERDA detectors are constructed, the materials used will be carefully assayed and characterized. All this information will be saved in a database as well. MAGE can then use this information to include the measured activities in the simulation on a component-by-component level, reducing systematic uncertainties in sensitivity calculations.

This design allows the simulation of detectors, prototypes and validation experiments to be performed within the same framework using the same physics processes, geometries and tools. This eases cross-comparisons and reduces coding and debugging effort.

IV. PHYSICS

The physics list in MAGE has been optimized for the reliable simulation of the signal process and the most common background sources in $0\nu\beta\beta$ -decay experiments. It was selected according to the suggestions of the GEANT4 team [15] and optimized for low-background physics applications [6], [16].

MAGE has a default physics list that is mainly based on the Underground Physics advanced example which

is distributed with GEANT4 [15]. The hadronic models implemented in the physics list are

- theory-driven quark-gluon string models (QGSP) for pions, kaons and nucleons with energies up to 100 TeV;
- low energy parameterized (LEP) models [7] for inelastic interactions of pions and nucleons with energies between 10 and 12 GeV, and for kaons below 25 GeV;
- Bertini (BERT) or, alternatively, Binary (BIC) cascade models are used to describe nucleon and pion interactions below energies of 10 GeV;
- data-driven neutron capture, fission, and elastic and inelastic scattering models from thermal energies to 20 MeV based on tabulated cross-section data derived from the ENDF/B-VI database [17] (HP models).

Alternative hadronic physics lists are available in MAGE that can be instantiated by messenger commands. Dedicated commands allow to use only LEP models (instead of cascades) for nucleons below 10 GeV, and to select Bertini or Binary models for nuclear cascades. For inelastic interactions of neutrons with energy below 8 GeV, it is also possible to use an alternative theory-driven quark-gluon string model (QGSC) which employs chiral-invariant phase-space modeling for nuclear de-excitation [7].

Interactions of leptons with nucleons are simulated using the equivalent photon approximation. Photonuclear interactions are modeled in detail and are divided into five energy regions:

- the giant dipole resonance region (10-30 MeV);
- the quasi-deuteron region (from 30 MeV to the pion production threshold);

- the Λ region (from the pion production threshold to 450 MeV);
- the Roper resonance region (450 MeV to 1.2 GeV);
- the Reggeon-Pomeron region (1.2-3.5 GeV).

Hadronic final states are generated using a chiral-invariant phase-space decay model. For energies above 3.5 GeV, photonuclear interactions are described by QGSP models.

Low-energy models [7] for the description of electromagnetic interactions of γ -rays, electrons and ions provided by GEANT4 are used in MAGE by default. These models include atomic effects (e.g. fluorescence and Doppler broadening) and can handle interactions down to energies of 250 eV. Synchrotron radiation is also included in the physics list for electrons and positrons. Alternatively, electromagnetic interactions of γ -rays, electrons and ions can be described by so-called standard models provided by GEANT4. These models are tuned to high-energy physics applications; they are less precise in the low-energy region and do not include atomic effects. However, they are faster in terms of computing time. The electromagnetic physics processes provided by GEANT4 for γ -rays and e^\pm (both standard and low-energy) have been systematically validated by the GEANT4 Collaboration [18] and by other groups [19] at the few-percent level. For the description of electromagnetic interactions of muons, only standard models are available in GEANT4.

MAGE takes advantage of GEANT4's ability to handle optical photons. While the default MAGE physics list does not include interactions of optical photons these processes can be enabled during runtime. The underlying models encompass scintillation light emission (possibly

with different light yields for electrons, α -particles and nuclei), Cherenkov light emission, absorption, boundary processes, Rayleigh scattering and wavelength shifting. If optical photon treatment is enabled, it is necessary to specify all relevant optical properties of interfaces and bulk materials (refraction index, absorption length, etc.) in the geometry definition.

GEANT4 tracks all simulated particles down to zero range, although various options exist to manually limit step size, track length, time-of-flight, and other parameters. Production cuts for δ -rays and for soft bremsstrahlung photons are expressed in spatial ranges and are internally converted into energy thresholds for the production of soft photons and δ -rays in the corresponding material. It is necessary to find a trade-off between accuracy and computing time in most applications. Therefore MAGE provides three production cut realms: DarkMatter, DoubleBeta and CosmicRays. The DarkMatter realm is used for high-precision simulations, especially related to background studies for dark matter applications: the cuts for γ -rays and betas are 5 μm and 0.5 μm , respectively, corresponding to a ~ 1 keV energy threshold in metallic germanium. The DoubleBeta realm (MAGE default) is suitable for signal and background studies related to double-beta decay, i.e. in the MeV energy-region: the range cut for betas is lowered to 0.1 mm, corresponding to a 100 keV threshold in metallic germanium. The CosmicRay realm is used for the simulation of extensive electromagnetic showers induced by cosmic ray muons. The cut-per-region approach is used in this setup. Sensitive regions are defined for which the production cuts are the same as for the DoubleBeta realm. They

are more relaxed everywhere else (5 cm for γ -rays and 1 cm for betas). By avoiding the precise tracking of particles in the inactive detector components, computing time is saved.

MAGE includes some provisions to improve agreement between simulation and experimental results. For instance, simulations do not account for inefficient conversion of germanium nuclei recoil energy to ionization energy. MAGE contains output classes that simulate this conversion inefficiency.

GEANT4 performs simulations on an event-by-event basis, where each event begins with the release of a particle from a generator, and ends when the interactions of the primary particle and its secondaries have finished. When long-lived radioactive decays occur, a single GEANT4 event may span many simulated years. Output classes in MAGE divide GEANT4 events into intervals that span user-selectable times. The total energy deposited during specific time intervals can be reported. This information can be used to simulate the effectiveness of timing cuts at removing backgrounds. It can also improve agreement between results of MAGE simulations and experimental data. Simulated energy deposits occurring long after the duration of an experiment can be excluded. Simulated energy deposits in close succession can be summed to approximate the pile-up due to the finite time resolution of data acquisition hardware used in an experiment.

V. EXAMPLE: LIQUID NITROGEN TEST STAND

The validation of the Monte Carlo code is an important step in the development of MAGE. This section presents the results of an auxiliary measurement performed in

the context of GERDA. It is an example of the validation procedure and shows the level of agreement between data and Monte Carlo prediction for a particular case.

The data used in the following comparison were obtained from a measurement of radioactive γ -sources with a germanium detector operated directly in a buffer of liquid nitrogen. The experimental setup is shown in Fig. 1.

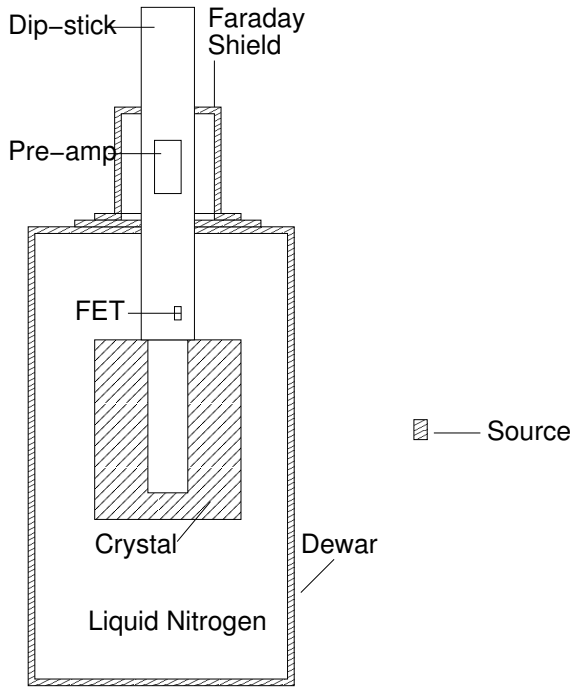


Fig. 1. Schematic drawing of the liquid nitrogen test stand. The germanium detector is mounted onto a dip-stick and submerged into a buffer of liquid nitrogen contained inside a double-walled aluminum cryostat.

The double-walled aluminum dewar containing the liquid nitrogen has a diameter of 203 mm and a height of 410 mm. The two walls are separated by 23.8 mm. The inner and outer wall thicknesses are 0.3 mm and 1.2 mm, respectively. The detector center is radially shifted by 17.7 mm from the center of the dewar.

The high-purity *n*-type germanium detector has a closed-ended coaxial geometry. It has a height of 77.2 mm and a diameter of 64.5 mm. The core electrode has a depth of 61 mm and a diameter of 10 mm. The dead layer on the outer mantle is due to boron implantation and has a thickness of about $0.3 \mu\text{m}$. It is shielded by an $0.3 \mu\text{m}$ thick aluminum layer. The inner dead layer is due to drifted lithium and has a thickness of approximately $600 \mu\text{m}$. The detector is operated at a voltage of 3.5 kV. The FET of the pre-amplifier is operated close to the detector inside the liquid nitrogen. The pre-amplifying electronics are located outside the dewar and within a copper Faraday shield. The DAQ energy threshold is set to 150 keV to avoid electronic noise from the pre-amplifier. A software cut on the energy is applied at 270 keV in order to avoid the low-energy region in which the trigger efficiency is decreasing with decreasing energy.

Measurements were performed with three radioactive sources, ^{60}Co , ^{152}Eu and ^{228}Th . The sources were placed at a radial distance of 10 cm from the dewar and vertically aligned with the center of the detector. An additional background measurement was performed without a source present. Around 1.4×10^6 events were collected in each measurement with a source present (source data sets); around 150,000 events were collected in the background data set.

The experimental setup was simulated using the MAGE framework built against GEANT4 version 8.2 with patch01 applied. About 10^8 events were simulated for each source. ^{60}Co decays were generated using

the GEANT4 generator G4ParticleGun neglecting the angular correlation between the emitted γ -rays. Earlier studies have shown that in similar geometries no statistically significant differences between ^{60}Co decays with and without angular correlation between the emitted γ -rays were observed. The energies obtained by the simulation were smeared according to the energy resolution measured with the detector. The energy threshold cuts applied to the measured data were also applied to Monte Carlo data.

In order to compare the measured data with Monte Carlo predictions the background from radioactivity in the laboratory is estimated for each source data set by scaling the background data set according to fits the number of events in characteristics γ -lines. The procedure is described in [20]. As an example the energy spectrum obtained from the ^{60}Co data set is shown in Fig. 2 together with the Monte Carlo-plus-background spectrum. The measured Compton continuum below 1.1 MeV is well described by the simulation. The average deviation in that region is approximately 5% with the data being systematically higher than the Monte Carlo plus background spectrum. The numbers of events under the two characteristic peaks of ^{60}Co at 1,173 keV and 1,332 keV are higher in Monte Carlo compared to measured data by about 10%. The spectrum is dominated by background events for higher energies. The disagreement between the measured and simulated data in this region is less than 15% on average with the data being systematically lower than the Monte Carlo plus background spectrum.

Fig. 3 shows the ratio of the number of events in

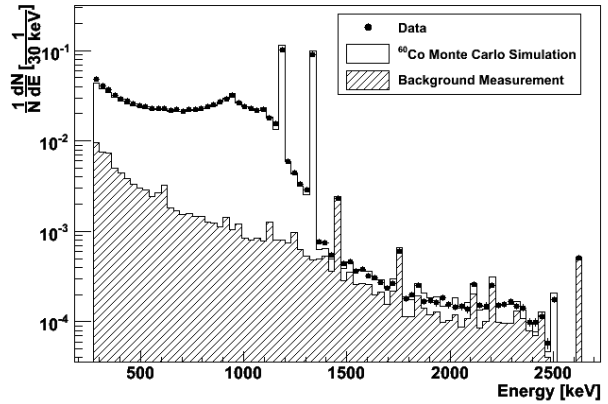


Fig. 2. Energy spectrum of the ^{60}Co data set. The measured data is represented by markers. The error bars show the statistical uncertainty. The Monte Carlo and background data sets are represented by the open and hatched histograms, respectively.

the data and Monte Carlo plus background samples for the 5σ -regions around the most prominent peaks. The markers indicate the statistical uncertainty. The Monte Carlo plus background data sets show a systematic excess of events which is slightly energy dependent. The excess ranges from 1% for an energy of 344.27 keV (^{152}Eu) up to 12% at an energy of 2614.53 keV (^{208}Tl in the ^{228}Th decay chain).

The overall agreement between the experimental data and the prediction from the simulation are on the 5-10% level. This is reasonable agreement given that the spectral shape and peak heights, which span four orders of magnitude in intensity, depend sensitively on geometric effects. Discrepancies likely arise particularly from

- insufficient modeling of the experimental setup. In Ref. [21] it has been shown that an agreement better than a few percent can be obtained for γ -ray interactions in HPGe detectors with GEANT4 by a proper

optimization of the model of the experimental setup;

- inefficiency effects which are not included in the simulation, such as pile-up, trigger turn-on and digitization.

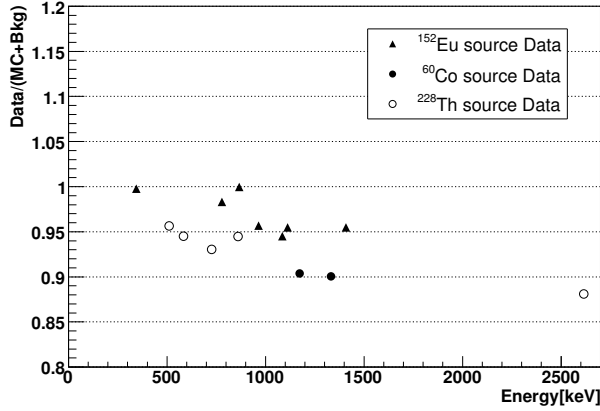


Fig. 3. Ratio of number of events in the data and Monte Carlo plus background samples for the most prominent peaks of ^{60}Co (filled circle), ^{152}Eu (triangle) and ^{228}Th (open circle). The statistical uncertainty is smaller than the marker size.

VI. VALIDATION OF THE SIMULATION

The GEANT4 simulation toolkit is used in various applications of modern physics. These range from simulations in high-energy particle physics to astrophysics and medical science. In parallel to the development of new simulation modules the verification of the simulation code is an important task for developers and users. Several modules have been developed to describe the interactions of low energy photons, electrons and hadrons with matter [22]. These are of particular importance for applications such as MAGE and are tested within the two collaborations developing the software. In the following, the current status of MAGE verification efforts is summarized.

The description of electromagnetic interactions in the energy region up to several MeV was tested with high-purity germanium detector systems, such as that presented in Section V. The most extensive verification effort was performed with a 18-fold segmented GERDA prototype detector. The segmented germanium crystal was operated and exposed to several radioactive sources (^{60}Co , ^{228}Th , ^{152}Eu) [20], [23]. A large fraction of the emitted gammas deposit energy in more than one segment. This feature allows these events to be distinguished from those which deposit energy in relatively small volumes, such as $0\nu\beta\beta$ -decays. Such segmentation-based discrimination between single- and multiple-site interactions was compared between experiment and simulation, with deviations found on the 5% level.

The description of neutron interactions with Ge is probed by comparing data from a measurement of an AmBe source with predictions from MAGE. The measurements have been performed with a CLOVER detector and with the 18-fold segmented detector described previously [24]. At an energy level of several MeV, neutrons mostly interact through elastic and inelastic scattering as well as neutron absorption. The measured energy spectra were studied and photon lines from neutron interactions with the germanium detector itself and the surrounding materials were identified [25]. Several discrepancies in the GEANT4 simulation were identified. The 2223.0-keV peak from $\text{H}(n,\gamma)\text{D}$ appears at 2224.6 keV in GEANT4 simulations (bug report # 955) [26]. This problem can be corrected by modifying data files provided with GEANT4. Meta-stable nuclear states are not produced by GEANT4 as a result of

neutron interactions (bug report # 956) [26]. The GEANT4 collaboration is investigating this issue. Neutrons also do not produce internal conversion electrons in GEANT4 (bug report # 957) [26]. MAGE developers are working towards a solution for this problem.

The MAGE package was also used to study and verify the simulation of spallation neutron production and propagation. At the CERN NA55 experiment the neutron production from a 190 GeV muon beam incident on different targets was measured. At the SLAC electron beam dump experiment the neutron propagation through different thicknesses of concrete was measured. Both experiments were simulated within the MAGE framework. It was found that MAGE/GEANT4 underestimate the neutron production from muon interactions measured by NA55, especially in high-Z materials, by more than a factor of two [27]. Results obtained in the MAGE simulation of NA55 have been compared with the GEANT4- and FLUKA-based [28] Monte Carlo simulations of the same experiment performed in [29], and found to be consistent. The disagreement between Monte Carlo simulation codes and NA55 data for muon-induced neutron production is discussed in detail in [29], [30]. The attenuation of the neutron propagation is found to be larger in the simulation than measured in the SLAC experiment [27]. A method to correct the neutron over-attenuation in MAGE-based simulations is described in [27].

VII. CONCLUSIONS

We presented the MAGE framework for simulating interactions in neutrinoless double-beta decay experiments that utilize enriched HPGe detectors. The benefits of MAGE can be summarized as:

- reliable Monte Carlo framework based on GEANT4 for low-background, low-energy experiments;
- ongoing tests of the code and validation of the physics processes;
- flexible geometry and physics application that emphasizes code reuse and verification;
- general purpose tools like surface and volume sampling, custom isotope decay generators, etc.

In general there is good agreement between the MAGE simulation and the measurements of electromagnetic interactions with average discrepancies of the order of (5-10)%. Several problems have been identified in the simulation of neutron interactions in GEANT4. These problems have been reported to the GEANT4 collaboration and are under investigation by the MAGE developers.

We anticipate that MAGE will form the foundation of the simulation and analysis framework of the GERDA and MAJORANA experiments. This framework is also applicable for other low-background underground experiments, such as solar, reactor and geological neutrino experiments, direct dark matter searches, and other neutrinoless double-beta decay search. These experiments share many detection techniques and background issues in common with GERDA and MAJORANA.

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